



UNIVERSITEIT VAN PRETORIA
UNIVERSITY OF PRETORIA
YUNIBESITHI YA PRETORIA

Contribution ID: 509

Type: **Poster Presentation**

Ab-initio Study of Elastic Properties of Ru-Cr and Pt-Cr Alloys

Thursday, 12 July 2012 17:30 (2 hours)

Abstract content
 (Max 300 words)

With the use of density functional theory, First principles planewave pseudopotential methods has been used to investigate the elastic properties of Pt-Cr and Ru-Cr binary alloys. The elastic constants, bulk modulus, shear modulus and Young's modulus were calculated for the different phases of the composition of A₃B and AB₃ (where A = Pt or Ru and B = Cr). The results provide useful information on elastic properties of PtCr binary alloys with promising application as coatings to cover the turbine engines which are exposed to aggressive environments.

Apply to be
 consider for a student
 award (Yes / No)?

no

Level for award
 (Hons, MSc,
 PhD)?

none

Would you like to
 submit a short paper
 for the Conference
 Pro-ceedings (Yes / No)?

no

Primary author: Dr TIBANE, Malebo (University of South Africa)

Co-author: Prof. NGOEPE, Phuti (University of Limpopo)

Presenter: Dr TIBANE, Malebo (University of South Africa)

Session Classification: Poster Session

Track Classification: Track A - Division for Condensed Matter Physics and Materials